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STRUCTURE FILE UPDATES: 7 JUN 2010   HIGHEST RN 1227141-97-0
DICTIONARY FILE UPDATES: 7 JUN 2010   HIGHEST RN 1227141-97-0

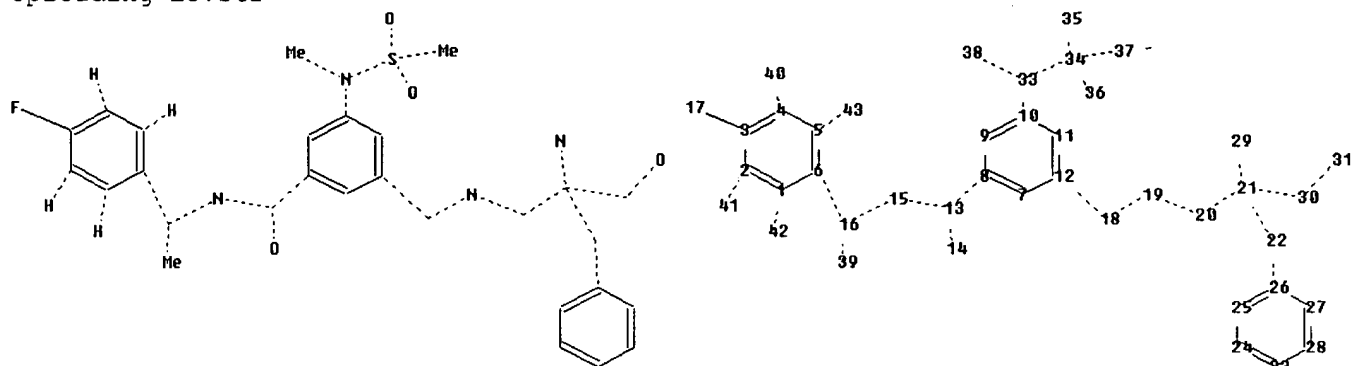New CAS Information Use Policies, enter HELP USAGETERMS for details.

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REGISTRY includes numerically searchable data for experimental and
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experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

http://www.cas.org/support/stngen/stndoc/properties.html
Uploading L3.str

chain nodes :
13   14   15   16   17   18   19   20   21   22   29   30   31   33   34   35   36   37   38   39   40
41   42   43
ring nodes :
1   2   3   4   5   6   7   8   9   10   11   12   23   24   25   26   27   28
chain bonds :
1-42   2-41   3-17   4-40   5-43   6-16   8-13   10-33   12-18   13-14   13-15   15-16   16-39
18-19   19-20   20-21   21-22   21-29   21-30   22-26   30-31   33-34   33-38   34-35   34-36
34-37
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   23-24   23-28   24-
25
25-26   26-27   27-28
exact/norm bonds :
1-42   2-41   4-40   5-43   6-16   8-13   10-33   12-18   13-14   13-15   15-16   16-39   18-19
19-20   20-21   21-22   21-29   21-30   22-26   30-31   33-34   33-38   34-35   34-36   34-37
exact bonds :
3-17
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   23-24   23-28   24-
25
25-26   26-27   27-28

Connectivity :
13:3 E exact RC ring/chain   14:1 E exact RC ring/chain   15:2 E exact RC ring/chain
18:2 E exact RC ring/chain   19:2 E exact RC ring/chain   20:2 E exact RC ring/chain

22:2 E exact
RC ring/chain 29:1 E exact RC ring/chain · 30:2 E exact RC ring/chain 31:1 E exact
RC ring/chain

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS
19:CLASS 20:CLASS 21:CLASS
22:CLASS 23:Atom 24:Atom 25:Atom 26:Atom 27:Atom 28:Atom 29:CLASS 30:CLASS
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43:CLASS

=> d stat que L5
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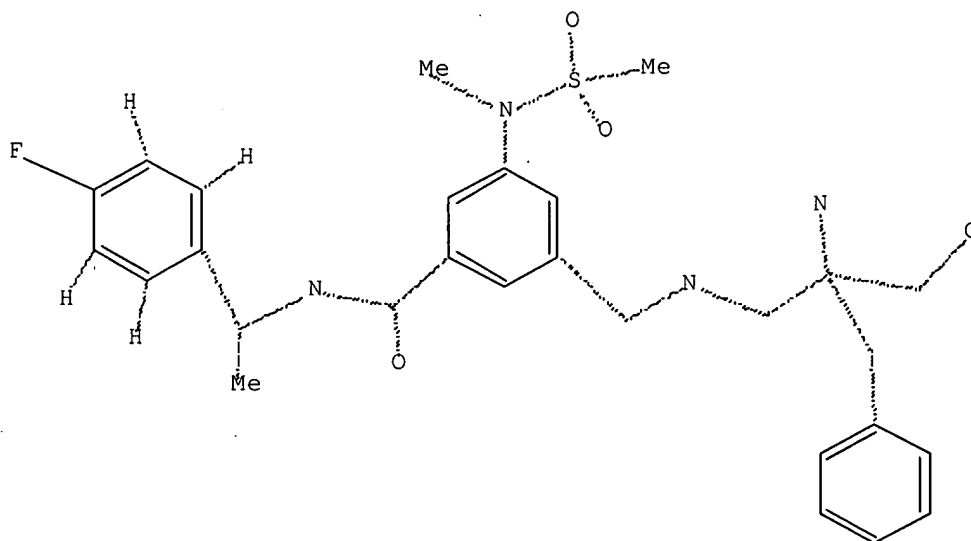
Structure attributes must be viewed using STN Express query preparation.
L5   3 SEA FILE=REGISTRY SSS FUL L3

100.0% PROCESSED   950 ITERATIONS   3 ANSWERS
SEARCH TIME: 00.00.01

=> file zcaplus
FILE 'ZCAPLUS' ENTERED AT 11:28:27 ON 08 JUN 2010
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FILE COVERS 1907 - 8 Jun 2010   VOL 152 ISS 24
FILE LAST UPDATED: 7 Jun 2010   (20100607/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

ZCAplus now includes complete International Patent Classification (IPC)
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This file contains CAS Registry Numbers for easy and accurate
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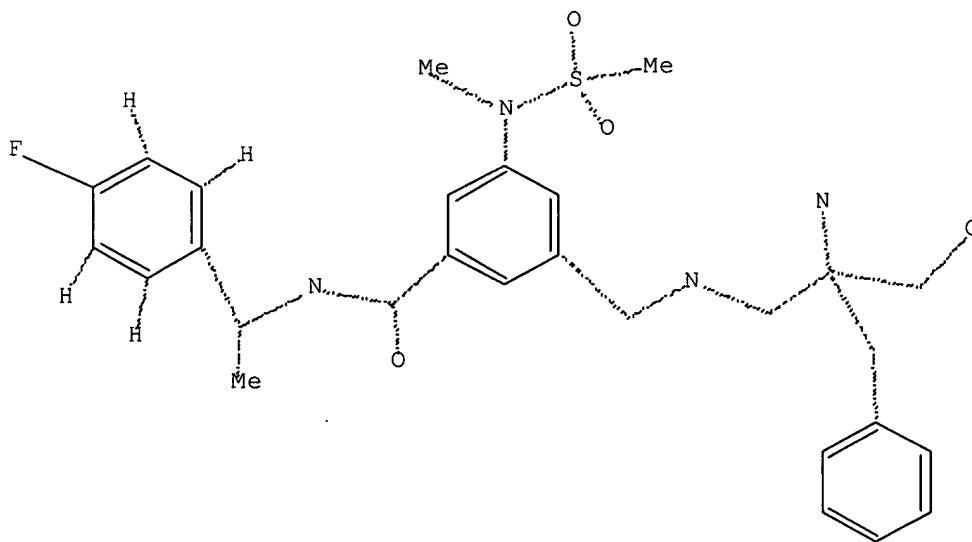

Structure attributes must be viewed using STN Express query preparation.
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L6         2 SEA FILE=ZCAPLUS SPE=ON   ABB=ON   PLU=ON   L5
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FILE 'BEILSTEIN' ENTERED AT 11:28:41 ON 08 JUN 2010
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FILE LAST UPDATED ON November 14, 2009
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10/573232

FILE COVERS 1779 TO 2009.
*** FILE CONTAINS 10,654,725 SUBSTANCES ***

>>>PLEASE NOTE: Reaction Data and substance data are stored in
   separate documents and can not be searched together in one query.
   Reaction data for BEILSTEIN compounds may be displayed
   immediately with the display codes PRE (preparations) and REA
   (reactions). A substance answer set retrieved after the search
   for a chemical name, a compounds with available reaction
   information by combining with PRE/FA, REA/FA or more generally
   with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
   between a BEILSTEIN compound and belonging reactions. For mo
   detailed reaction searches BRNs can be searched as reaction
   partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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* ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.   *
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    http://www.stn-international.com/stn_chemistry_beilstein.html

=> d stat que L8
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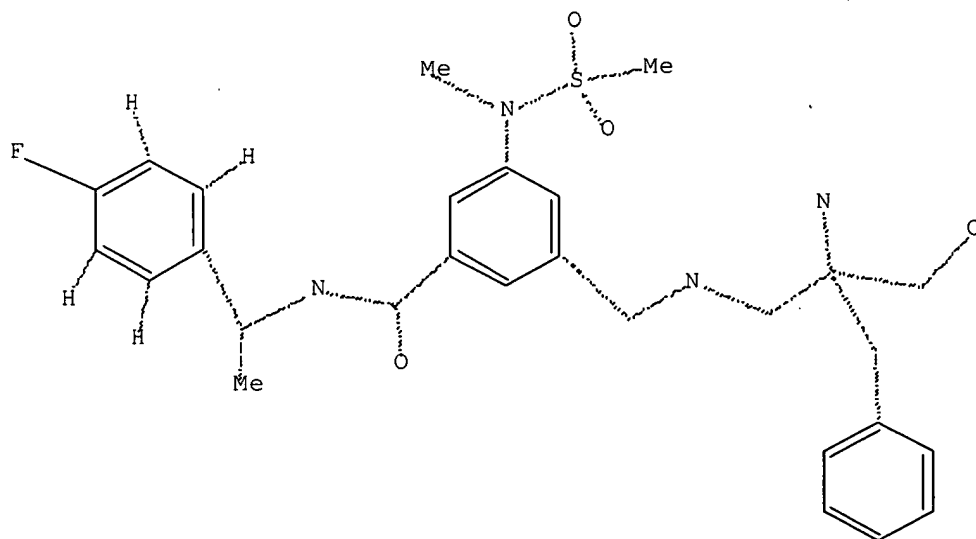
Structure attributes must be viewed using STN Express query preparation.
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100.0% PROCESSED   0 ITERATIONS   0 ANSWERS
SEARCH TIME: 00.00.02

5

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FILE LAST UPDATED:        4 JUN 2010    <20100604/UP>
MOST RECENT UPDATE:        201035       <201035/DW>
DERWENT WORLD PATENTS INDEX SUBSCRIBER FILE, COVERS 1963 TO DATE
>>> Now containing more than 1.5 million chemical structures in DCR <<<

>>> IPC, ECLA, US National Classifications and Japanese F-Terms
    and FI-Terms have been updated with reclassifications to
    end of March 2010.
    No update date (UP) has been created for the reclassified
    documents, but they can be identified by
    specific update codes (see HELP CLA for details) <<<

>>> FOR THE LATEST DERWENT WORLD PATENTS INDEX (DWPI)
    STN USER DOCUMENTATION, PLEASE VISIT:
    http://www.stn-international.com/stn_dwpi.html <<<

>>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

>>> For changes in DWPI see HELP CHANGE - last updated April 6, 2010 <<<

>>> New display format ALLSTR available - see NEWS  <<<

>>> US National Patent Classification thesaurus added - see NEWS <<<
'BIX' IS DEFAULT SEARCH FIELD FOR 'WPIX' FILE

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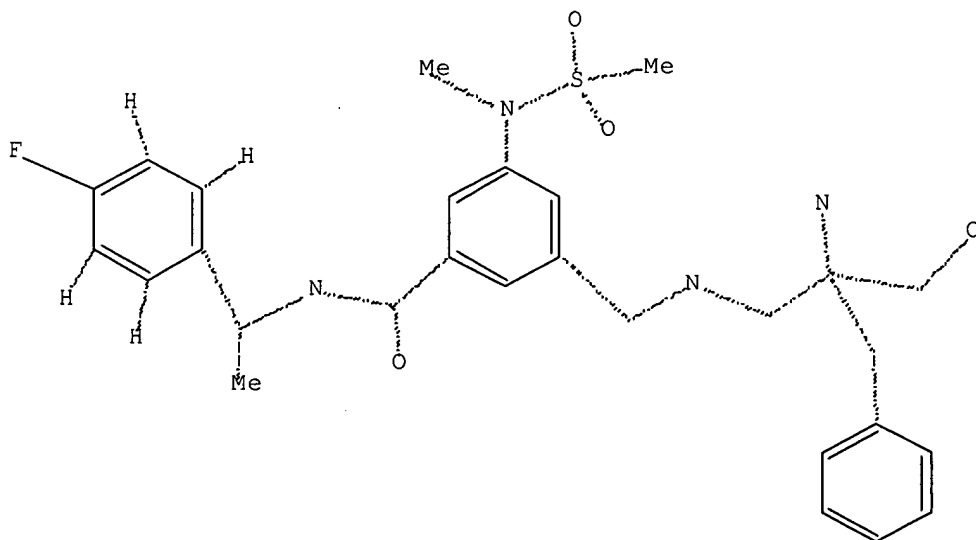


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Structure attributes must be viewed using STN Express query preparation.
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L11   1 SEA FILE=WPIX SPE=ON ABB=ON PLU=ON L10/DCR

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PROCESSING COMPLETED FOR L6
PROCESSING COMPLETED FOR L11
L12   2 DUP REM L6 L11 (1 DUPLICATE REMOVED)
                 ANSWERS '1-2' FROM FILE ZCAPLUS

=> d ibib abs hitstr L12 1-2

L12 ANSWER 1 OF 2   ZCAPLUS   COPYRIGHT 2010 ACS on STN DUPLICATE 1
ACCESSION NUMBER: 2005:324002 ZCAPLUS <u>Full-text</u>
DOCUMENT NUMBER: 142:373552
TITLE: Benzyl ethers and benzylamines as beta-secretase
                        inhibitors, their preparation and use for the
                        treatment of Alzheimer's disease
INVENTOR(S):   Nantermet, Philippe G.; Rajapakse, Hemaka Anthony;
                        Selnick, Harold G.
PATENT ASSIGNEE(S):   Merck & Co., Inc., USA
SOURCE: PCT Int. Appl., 47 pp.
                        CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

        PATENT NO.   KIND   DATE   APPLICATION NO.   DATE
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        WO 2005032471   A3   20050707
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                CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
                GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
                LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
                NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
                TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
           RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM,
                AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
                EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
                SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
                SN, TD, TG
        AU 2004277981   A1   20050414 AU 2004-277981   20040929
        AU 2004277981   B2   20091001
        CA 2540452   A1   20050414 CA 2004-2540452   20040929
        EP 1673078   A2   20060628 EP 2004-789263   20040929
        EP 1673078   B1   20080528
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        JP 2007507515   T   20070329 JP 2006-534062   20040929
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        IN 2006DN01546   A   20070810 IN 2006-DN1546   20060322

US 20060293380   A1   20061228   US 2006-573232   20060323
PRIORITY APPLN. INFO.:   US 2003-508369P   P   20031003
                                                WO 2004-US32009   W   20040929
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S):   MARPAT 142:373552
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB   The invention relates to a group of benzyl ethers and benzylamines I which are
      inhibitors of the beta-secretase enzyme. In compds. I, X is O or NH; Y is CH
      or N; R1 is selected from aryl, arylmethyl, heterocyclyl, and
      heterocyclylmethyl, wherein the ring is unsubstituted or substituted with one
      or more substituents selected from halo, OH, C1-6 alkyl, C2-6 alkenyl, C2-6
      alkynyl, cyano, and C1-6 alkoxy; R2 is selected from
      alkyl(alkylsulfonyl)amino, (alkylsulfonyl)amino, o-cyanophenyl, and, gem-
      cyanocycloalkyl; R3 is selected from (un)substituted (arylalkyl)aminocarbonyl,
      aminocarbonyl, alkylaminocarbonyl, cyclopropylethenyl, cyclopropylmethyloxy,
      and cyclopropylmethylamino; and includes all pharmaceutically acceptable
      salts. The invention also relates to the preparation of I, pharmaceutical
      compns. comprising these compds. and a pharmaceutically acceptable carrier,
      and the use of these compds. and compns. in the treatment of diseases in which
      the beta-secretase enzyme is involved, such as Alzheimer's disease. N-
      Methylsulfonylation of di-Me 5-aminoisophthalate, followed by N-methylation,
      gave II, which was partially hydrolyzed and coupled with a chiral amine to
      give III. Hydrolysis of III followed by borane reduction, bromination, and
      substitution with 2-amino-2-benzylpropane-1,3-diol, prepared by reduction of
      racemic α-benzylserine, resulted in the formation of IV. The compds. of the
      invention inhibit the beta-secretase enzyme, generally with IC50 values from
      about 1 nM to 100 μM.
IT   849623-02-5P, 3-[[(2-Amino-2-benzyl-3-
      hydroxypropyl)amino]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-
      [methyl(methylsulfonyl)amino]benzamide trifluoroacetate
      RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
      (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
      (Uses)
         (drug candidate; preparation of benzyl ethers and benzylamines as
      beta-secretase inhibitors for the treatment of Alzheimer's disease)
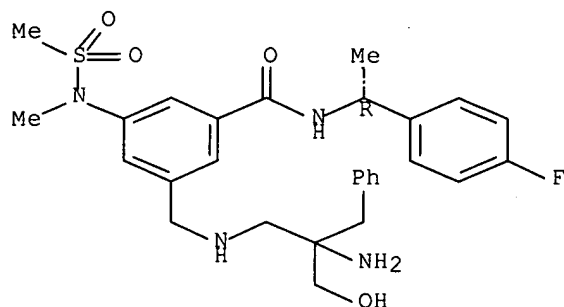RN   849623-02-5 ZCAPLUS
CN   Benzamide, 3-[[[2-amino-2-(hydroxymethyl)-3-phenylpropyl]amino]methyl]-N-
      [(1R)-1-(4-fluorophenyl)ethyl]-5-[methyl(methylsulfonyl)amino]-,
      2,2,2-trifluoroacetate (1:2) (CA INDEX NAME)

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      CRN   849623-01-4
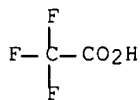   CMF   C28 H35 F N4 O4 S

Absolute stereochemistry.

CM   2

CRN   76-05-1
CMF   C2 H F3 O2

L12 ANSWER 2 OF 2 ZCAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2010:295671 ZCAPLUS Full-text
DOCUMENT NUMBER: 152:516542
TITLE: SAR of tertiary carbinamine derived BACE1 inhibitors:
                           Role of aspartate ligand amine pK a in enzyme
                           inhibition
AUTHOR(S):   Rajapakse, Hemaka A.; Nantermet, Philippe G.; Selnick,
                           Harold G.; Barrow, James C.; McGaughey, Georgia B.;
                           Munshi, Sanjeev; Lindsley, Stacey R.; Young, Mary
                           Beth; Ngo, Phung L.; Katherine Holloway, M.; Lai,
                           Ming-Tain; Espeseth, Amy S.; Shi, Xiao-Ping; Colussi,
                           Dennis; Pietrak, Beth; Crouthamel, Ming-Chih;
                           Tugusheva, Katherine; Huang, Qian; Xu, Min; Simon,
                           Adam J.; Kuo, Lawrence; Hazuda, Daria J.; Graham,
                           Samuel; Vacca, Joseph P.
CORPORATE SOURCE: Department of Medicinal Chemistry, Merck Research
                           Laboratories, West Point, PA, 19486, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (2010),
                           20(6), 1885-1889
                           CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB   The optimization of tertiary carbinamine derived inhibitors of BACE1 from its
     discovery as an unstable lead to low nanomolar cell active compds. is

described. Five-membered heterocycles are reported as stable and potency
enhancing linkers. In the course of this work, we have discovered a clear
trend where the activity of inhibitors at a given assay pH is dependent on pK
a of the amino group that interacts directly with the catalytic aspartates.
The potency of compds. as inhibitors of Aβ production in a cell culture assay
correlated much better with BACE1 enzyme potency measured at pH 7.5 than at pH
4.5.

IT   1225027-40-6
      RL: DMA (Drug mechanism of action); PAC (Pharmacological activity); THU
      (Therapeutic use); BIOL (Biological study); USES (Uses)
          (tertiary carbinamine-derived BACE1 inhibitors preparation and role of
          aspartate ligand amine pK a in enzyme inhibition)
RN   1225027-40-6 ZCAPLUS
CN   Benzamide, 3-[[[(2R)-2-amino-2-(hydroxymethyl)-3-
      phenylpropyl]amino]methyl]-N-[(1R)-1-(4-fluorophenyl)ethyl]-5-
      [methyl(methylsulfonyl)amino]- (CA INDEX NAME)

Absolute stereochemistry.
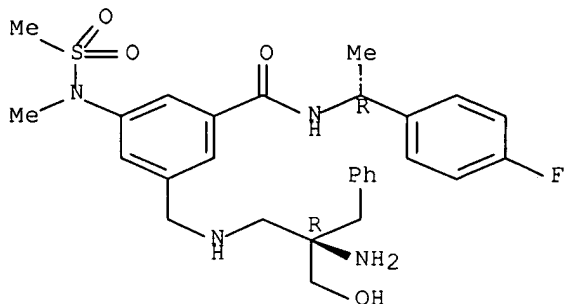
REFERENCE COUNT: 13   THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS
                                 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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=> d his full

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L2           0 SEA SSS SAM L1
L3               STRUCTURE UPLOADED
L4           0 SEA SSS SAM L3
L5           3 SEA SSS FUL L3
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L6           2 SEA SPE=ON  ABB=ON   PLU=ON   L5

     FILE 'BEILSTEIN' ENTERED AT 11:27:10 ON 08 JUN 2010
L7           0 SEA SSS SAM L3
L8           0 SEA SSS FUL L3

     FILE 'WPIX' ENTERED AT 11:27:26 ON 08 JUN 2010
L9           0 SEA SSS SAM L3
L10          1 SEA SSS FUL L3
L11          1 SEA SPE=ON  ABB=ON   PLU=ON   L10/DCR

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     FILE 'ZCAPLUS' ENTERED AT 11:28:27 ON 08 JUN 2010
                 D STAT QUE L6

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                 D STAT QUE L8

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                 D STAT QUE L11

     FILE 'ZCAPLUS, WPIX' ENTERED AT 11:29:04 ON 08 JUN 2010
L12          2 DUP REM L6 L11 (1 DUPLICATE REMOVED)
                   ANSWERS '1-2' FROM FILE ZCAPLUS
             D IBIB ABS HITSTR L12 1-2


     FILE HOME

     FILE REGISTRY
     Property values tagged with IC are from the ZIC/VINITI data file
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FILE ZCAPLUS

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FILE COVERS 1907 - 8 Jun 2010 VOL 152 ISS 24
FILE LAST UPDATED: 7 Jun 2010 (20100607/ED)
REVISED CLASS FIELDS (/NCL) LAST RELOADED: Apr 2010
USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Apr 2010

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This file contains CAS Registry Numbers for easy and accurate substance identification.

FILE BEILSTEIN
FILE LAST UPDATED ON November 14, 2009

FILE COVERS 1779 TO 2009.
 FILE CONTAINS 10,654,725 SUBSTANCES

>>>PLEASE NOTE: Reaction Data and substance data are stored in
    separate documents and can not be searched together in one query.
    Reaction data for BEILSTEIN compounds may be displayed
    immediately with the display codes PRE (preparations) and REA
    (reactions). A substance answer set retrieved after the search
    for a chemical name, a compounds with available reaction
    information by combining with PRE/FA, REA/FA or more generally
    with RX/FA. The BEILSTEIN Registry Number (BRN) is the link
    between a BEILSTEIN compound and belonging reactions. For mo
    detailed reaction searches BRNs can be searched as reaction
    partner BRNs Reactant BRN (RX.RBRN) or Product BRN (RX.PBRN).<<<

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    * ESTIMATES MAY NOT REFLECT THE ACTUAL COSTS.                        .*
    * FOR PRICE INFORMATION SEE HELP COST                                *
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    FILE WPIX
    FILE LAST UPDATED:        4 JUN 2010    <20100604/UP>
    MOST RECENT UPDATE:          201035     <201035/DW>
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        and FI-Terms have been updated with reclassifications to
        end of March 2010.
        No update date (UP) has been created for the reclassified
        documents, but they can be identified by
        specific update codes (see HELP CLA for details) <<<

    >>> FOR THE LATEST DERWENT WORLD PATENTS INDEX (DWPI)
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        http://www.stn-international.com/stn_dwpi.html <<<

    >>> HELP for European Patent Classifications see HELP ECLA, HELP ICO <<<

    >>> For changes in DWPI see HELP CHANGE - last updated April 6, 2010 <<<

    >>> New display format ALLSTR available - see NEWS  <<<

    >>> US National Patent Classification thesaurus added - see NEWS <<<

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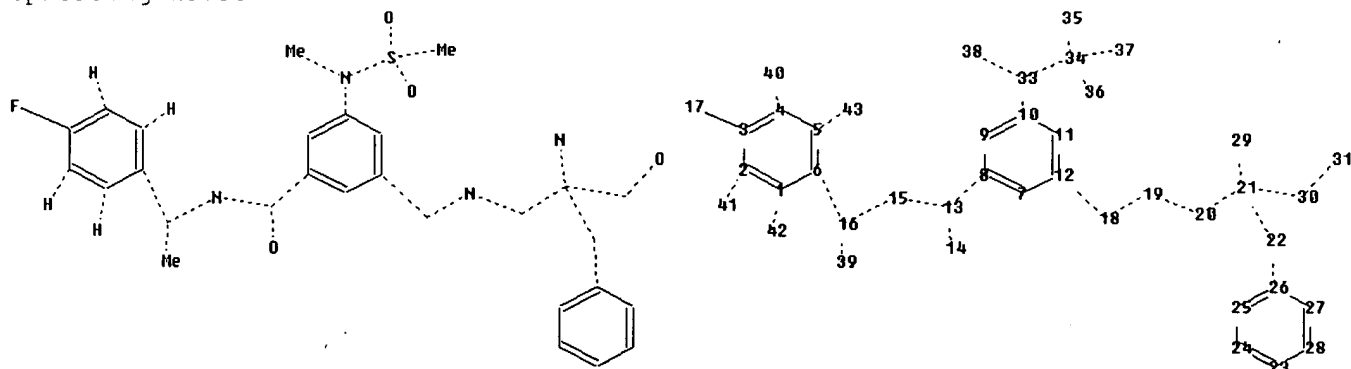


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chain nodes :
13   14   15   16   17   18   19   20   21   22   29   30   31   33   34   35   36   37   38   39   40
41   42   43
ring nodes :
1   2   3   4   5   6   7   8   9   10   11   12   23   24   25   26   27   28
chain bonds :
1-42   2-41   3-17   4-40   5-43   6-16   8-13   10-33   12-18   13-14   13-15   15-16   16-39
18-19   19-20   20-21   21-22   21-29   21-30   22-26   30-31   33-34   33-38   34-35   34-36
34-37
ring bonds :
1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   23-24   23-28   24-
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25
25-26  26-27  27-28
exact/norm bonds :
1-42   2-41   4-40   5-43   6-16   8-13   10-33   12-18   13-14   13-15   15-16   16-39   18-19
19-20   20-21   21-22   21-29   21-30   22-26   30-31   33-34   33-38   34-35   34-36   34-37
exact bonds :
3-17
normalized bonds :
1-2   1-6   2-3   3-4   4-5   5-6   7-8   7-12   8-9   9-10   10-11   11-12   23-24   23-28   24-
25
25-26   26-27   27-28
```

```
Connectivity :
13:3 E exact RC ring/chain   14:1 E exact RC ring/chain   15:2 E exact RC ring/chain
18:2 E exact RC ring/chain   19:2 E exact RC ring/chain   20:2 E exact RC ring/chain
22:2 E exact
RC ring/chain   29:1 E exact RC ring/chain   30:2 E exact RC ring/chain   31:1 E exact
RC ring/chain
```

```
Match level :
1:Atom   2:Atom   3:Atom   4:Atom   5:Atom   6:Atom   7:Atom   8:Atom   9:Atom   10:Atom
11:Atom   12:Atom   13:CLASS   14:CLASS   15:CLASS   16:CLASS   17:CLASS   18:CLASS
19:CLASS   20:CLASS   21:CLASS
22:CLASS   23:Atom   24:Atom   25:Atom   26:Atom   27:Atom   28:Atom   29:CLASS   30:CLASS
31:CLASS
33:CLASS   34:CLASS   35:CLASS   36:CLASS   37:CLASS   38:CLASS   39:CLASS   40:CLASS
41:CLASS   42:CLASS
43:CLASS
```